

Quadrupole transitions in the bound rotational-vibrational spectrum of the tritium molecular ion

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The nonrelativistic energies of the homonuclear ion T_2^+ are calculated for the ground state using the Lagrange-mesh method as was done for the isotopomers H_2^+ and D_2^+ (*J. Phys. B: At. Mol. Opt. Phys.* **45** 065101 and *J. Phys. B: At. Mol. Opt. Phys.* **46** 245101). Energies and eigenfunctions are obtained up to four of the lowest bound vibrational states ($v = 0, 1, 2, 3$) which support 62, 61, 60 and 58 bound rotational states, respectively. Some quasibound states are also presented until $L = 68$. From the obtained wave functions, electric quadrupole transitions per time unit are calculated between those states over the whole rotational bands. Extensive results are presented with 6 significant digits. The ground state energy of the symmetric systems ${}^\infty H_2^+$, ${}^\infty H^-$, Ps^- , H^- , D^- , T^- , $\mu^+ \mu^+ e$ and $\mu^+ e e$ is presented with high accuracy as a function of $\beta = m_3/(2m + m_3)$.

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INTRODUCTION

The molecular ion T_2^+ composed of two tritium nuclei (tritons) and one electron is the heaviest isotopomer of H_2^+ . This three body system is the less studied molecular ion in the family of three-body molecular systems with Coulomb interaction composed of protons, deuterons, tritons and one electron. A complete quantitative description has been done in some papers mainly for the ground state ($v = 0$ and $L = 0$). For this state, a complete list of various geometrical and energetically properties were obtained by Frolov [1, 2]. Polarizabilities and energies were calculated with high precision by Yan et al. [3] not only for the ground state but also for the lowest P state. In 2004 Yan et al. [4] reported non relativistic energies for those states with vibrational quantum number $v = 0$ and L ranging from 2 to 12. However, at present time, the number of rotational-vibrational bound states supported by the ground state is not known.

The goal of this paper is to present a systematic description of the spectra for the lowest four vibrational states $v = 0, 1, 2, 3$ and all the bound rotational states without considering the Born-Oppenheimer approximation. A few rotational states beyond the dissociation limit are also presented. In order to do that the Lagrange mesh method is applied in the same way that was done for the homonuclear systems H_2^+ [5] and D_2^+ [6]. This method is an approximate variational calculation using a basis of Lagrange functions and the associated Gauss quadrature. The main advantage of this method is its simplicity and high accuracy in the obtained energies and wave functions. With the analytical approximations for the wave functions provided by the Lagrange-mesh method allowed quadrupole transition probabilities are calculated. The CODATA 1986 fundamental constant $m_t = 5496.921\,58\,m_e$ is used.

Because this method was applied successfully for the three body systems with Coulomb interaction H_2^+ [5], D_2^+ [6] and HD^+ [7] the reader is referred to these references for details. In Sec. I only the expression for the quadrupole transition is presented. In Sec. II, energies are given for the lowest four vibrational levels over the full rotational bands and E2 transition probabilities are tabulated. Concluding remarks are presented in Sec. III. Throughout atomic units are used.

I. QUADRUPOLE TRANSITION PROBABILITIES

The electric quadrupole transition probability for spontaneous emission ($E_f < E_i$) per time unit (the atomic unit of time is $a_0/\alpha c \approx 2.4188843 \times 10^{-17} s$) between an initial state i and a final state f is given by

$$W_{i \rightarrow f}^{(2)} = \frac{1}{15} \alpha^5 (E_i - E_f)^5 \frac{S_{if}^{(2)}}{2J_i + 1}, \quad (1)$$

where α is the fine-structure constant, $S_{if}^{(2)}$ is the reduced matrix element and J_i the total angular momentum of the initial state. The quadrupole oscillator strength is given by

$$f_{i \rightarrow f}^{(2)} = \frac{1}{30} \alpha^2 (E_f - E_i)^3 \frac{S_{if}^{(2)}}{2J_i + 1}. \quad (2)$$

The evaluation of the reduced matrix element $S_{if}^{(2)}$ makes necessary to have the wave functions of the final and initial states. In our approximation, the wave functions are obtained using the Lagrange-mesh method. In order to apply this method, we use the center of mass coordinates. The six-dimensional wave function is presented as a product of two three-dimensional functions, (i) a function carrying all the angular dependence, and (ii) a function describing the form of the triangle formed by the three particles. For this internal degrees of freedom, the function is expanded in a three-dimensional Lagrange functions which are nothing but a product of three one-dimension Lagrange functions. The size of each one-dimensional bases are indicated by N_x , N_y and N_z . Because of the symmetry between the two centers $N_x = N_y \equiv N$. Three additional parameters h_x , h_y and h_z are introduced in order to adjust the base to the physical problem. Due to the symmetry between the two centers $h_x = h_y \equiv h$. Any state is labeled by the total angular momentum L , the vibrational quantum number v and the parity π : (L^π, v) . For a detailed discussion see [5–7].

II. T_2^+ BOUND AND QUASIBOUND ENERGIES

The rotational-vibrational spectra of the molecular ion T_2^+ is obtained using the Lagrange mesh method. Energies for the four lowest vibrational states ($v = 0, 1, 2, 3$) of the ground electronic state are presented in Table I. An important part of this work is to obtain the quadrupole transition probability per time unit, then, it is convenient to use a single three-dimensional mesh for all states. An excellent accuracy is obtained when the size of the bases

are chosen as $N = 54$ and $N_z = 18$ and the scaling parameters as $h = 0.08$ and $h_z = 0.6$. In this paper the triton mass value $m_t = 5496.921\,58\,m_e$ is used. The dissociation energy is then at $E_d = -0.499\,909\,056\,5$ a.u. The first line for each L -value in Table I presents the obtained energies. Comparison with previous results are possible only for the lowest twelve rotational states with vibrational quantum number $v = 0$. The energy for the ground state $(0^+, 0)$ is well known and our result is in agreement in 13 significant digits with the most accurate results presented by Frolov [2] and Yan *et al* [3]. The first rotational state $(1^-, 0)$ was studied also by Yan *et al* [3] and the agreement is in the 13 significant digit. Energies of the excited states $(L^\pi, 0)$ for $L \in (2, 12)$ are reported by Yan *et al* [4] and all of them have the same correspondence of 13 significant digits with our results.

Convergence for the energies was tested by changing the values of N and N_z . The accuracies for the first, second and third rotational bands are 10^{-11} , 10^{-10} and 10^{-9} , respectively. The results demonstrate that the vibrational band with quantum number $v = 0$ supports 62 rotational states below the dissociation energy. The number of rotational states below the dissociation energy supported by excited vibrational bands decrease with the vibrational quantum number: 61, 60 and 58 for $v = 1, 2, 3$, respectively. The obtained spectrum is depicted in Figure 1.

TABLE I: Energies of the four lowest vibrational bound or quasibound states in the Σ_g rotational band of the T_2^+ molecular ion. Quasibound states are separated from bound states by a horizontal bar. For each L value the first line presents the Lagrange-mesh results obtained with $N_x = N_y = 54$, $N_z = 18$ and $h_x = h_y = 0.08$, $h_z = 0.6$. More accurate energies are given for some levels (a: [2], b:[3], c: [4]). The triton mass is taken as $m_t = 5496.92158\,m_e$.

| L | $v = 0$ | $v = 1$ | $v = 2$ | $v = 3$ |
|-----|-------------------------------------|--------------------|-------------------|------------------|
| 0 | -0.599 506 910 111 5 | -0.593 589 927 812 | -0.587 871 233 66 | -0.582 346 606 1 |
| | -0.599 506 910 111 54 ^a | | | |
| | -0.599 506 910 111 541 ^b | | | |

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TABLE I – Continuation

| L | $v = 0$ | $v = 1$ | $v = 2$ | $v = 3$ |
|-----|---|--------------------|-------------------|------------------|
| 1 | -0.599 417 152 359 8 -0.599 417 152 359 852 ^b | -0.593 502 913 068 | -0.587 786 903 36 | -0.582 264 906 3 |
| 2 | -0.599 237 876 293 2 -0.599 237 876 293 205 ^c | -0.593 329 117 147 | -0.587 618 470 66 | -0.582 101 729 3 |
| 3 | -0.598 969 558 697 0 -0.598 969 558 696 973 ^c | -0.593 069 005 140 | -0.587 366 389 36 | -0.581 857 517 8 |
| 4 | -0.598 612 909 571 6 -0.598 612 909 571 611 ^c | -0.592 723 269 598 | -0.587 031 335 15 | -0.581 532 931 3 |
| 5 | -0.598 168 866 037 2 -0.598 168 866 037 205 ^c | -0.592 292 824 563 | -0.586 614 199 81 | -0.581 128 840 1 |
| 6 | -0.597 638 584 397 7 -0.597 638 584 397 716 ^c | -0.591 778 797 787 | -0.586 116 083 51 | -0.580 646 317 7 |
| 7 | -0.597 023 430 520 0 -0.597 023 430 520 051 ^c | -0.591 182 521 300 | -0.585 538 285 67 | -0.580 086 632 0 |
| 8 | -0.596 324 968 711 3 -0.596 324 968 711 257 ^c | -0.590 505 520 522 | -0.584 882 294 18 | -0.579 451 235 0 |
| 9 | -0.595 544 949 299 1 -0.595 544 949 299 086 ^c | -0.589 749 502 104 | -0.584 149 773 62 | -0.578 741 750 4 |
| 10 | -0.594 685 295 136 5 -0.594 685 295 136 511 ^c | -0.588 916 340 727 | -0.583 342 552 27 | -0.577 959 962 1 |
| 11 | -0.593 748 087 259 4 -0.593 748 087 259 376 ^c | -0.588 008 065 087 | -0.582 462 608 44 | -0.577 107 799 7 |
| 12 | -0.592 735 549 928 4 -0.592 735 549 928 400 ^c | -0.587 026 843 285 | -0.581 512 056 21 | -0.576 187 325 4 |
| 13 | -0.591 650 035 282 8 | -0.585 974 967 849 | -0.580 493 130 81 | -0.575 200 719 5 |
| 14 | -0.590 494 007 823 0 | -0.584 854 840 613 | -0.579 408 173 90 | -0.574 150 265 8 |
| 15 | -0.589 270 028 927 2 | -0.583 668 957 635 | -0.578 259 618 84 | -0.573 038 337 6 |

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TABLE I – Continuation

| $L \ v = 0$ | $v = 1$ | $v = 2$ | $v = 3$ |
|-------------------------|--------------------|-------------------|------------------|
| 16 -0.587 980 741 586 5 | -0.582 419 894 344 | -0.577 049 976 31 | -0.571 867 383 5 |
| 17 -0.586 628 855 526 3 | -0.581 110 291 083 | -0.575 781 820 19 | -0.570 639 913 7 |
| 18 -0.585 217 132 856 0 | -0.579 742 839 179 | -0.574 457 774 08 | -0.569 358 487 3 |
| 19 -0.583 748 374 370 8 | -0.578 320 267 657 | -0.573 080 498 44 | -0.568 025 699 1 |
| 20 -0.582 225 406 601 3 | -0.576 845 330 704 | -0.571 652 678 40 | -0.566 644 168 6 |
| 21 -0.580 651 069 688 7 | -0.575 320 795 939 | -0.570 177 012 45 | -0.565 216 528 3 |
| 22 -0.579 028 206 140 4 | -0.573 749 433 558 | -0.568 656 201 95 | -0.563 745 414 4 |
| 23 -0.577 359 650 502 1 | -0.572 134 006 365 | -0.567 092 941 54 | -0.562 233 456 7 |
| 24 -0.575 648 219 963 7 | -0.570 477 260 739 | -0.565 489 910 42 | -0.560 683 270 9 |
| 25 -0.573 896 705 902 6 | -0.568 781 918 497 | -0.563 849 764 56 | -0.559 097 450 9 |
| 26 -0.572 107 866 354 7 | -0.567 050 669 681 | -0.562 175 129 76 | -0.557 478 562 0 |
| 27 -0.570 284 419 389 4 | -0.565 286 166 215 | -0.560 468 595 63 | -0.555 829 135 2 |
| 28 -0.568 429 037 360 5 | -0.563 491 016 423 | -0.558 732 710 35 | -0.554 151 662 7 |
| 29 -0.566 544 341 992 9 | -0.561 667 780 362 | -0.556 969 976 24 | -0.552 448 592 9 |
| 30 -0.564 632 900 264 8 | -0.559 818 965 926 | -0.555 182 846 09 | -0.550 722 327 7 |
| 31 -0.562 697 221 036 4 | -0.557 947 025 683 | -0.553 373 720 25 | -0.548 975 219 3 |
| 32 -0.560 739 752 377 7 | -0.556 054 354 391 | -0.551 544 944 28 | -0.547 209 568 5 |
| 33 -0.558 762 879 545 2 | -0.554 143 287 149 | -0.549 698 807 35 | -0.545 427 622 9 |
| 34 -0.556 768 923 558 7 | -0.552 216 098 133 | -0.547 837 541 08 | -0.543 631 576 1 |
| 35 -0.554 760 140 328 2 | -0.550 274 999 878 | -0.545 963 319 07 | -0.541 823 567 5 |
| 36 -0.552 738 720 285 9 | -0.548 322 143 055 | -0.544 078 256 80 | -0.540 005 682 4 |
| 37 -0.550 706 788 477 6 | -0.546 359 616 697 | -0.542 184 412 02 | -0.538 179 952 4 |
| 38 -0.548 666 405 072 7 | -0.544 389 448 859 | -0.540 283 785 61 | -0.536 348 356 7 |
| 39 -0.546 619 566 254 9 | -0.542 413 607 645 | -0.538 378 322 77 | -0.534 512 823 4 |
| 40 -0.544 568 205 458 6 | -0.540 434 002 600 | -0.536 469 914 65 | -0.532 675 231 4 |
| 41 -0.542 514 194 920 6 | -0.538 452 486 430 | -0.534 560 400 24 | -0.530 837 412 8 |
| 42 -0.540 459 347 520 8 | -0.536 470 857 022 | -0.532 651 568 69 | -0.529 001 155 2 |

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TABLE I – Continuation

| $L \ v = 0$ | $v = 1$ | $v = 2$ | $v = 3$ |
|-------------------------|--------------------|-------------------|------------------|
| 43 -0.538 405 418 889 7 | -0.534 490 859 764 | -0.530 745 161 89 | -0.527 168 205 1 |
| 44 -0.536 354 109 765 3 | -0.532 514 190 143 | -0.528 842 877 46 | -0.525 340 271 0 |
| 45 -0.534 307 068 587 2 | -0.530 542 496 620 | -0.526 946 371 95 | -0.523 519 027 4 |
| 46 -0.532 265 894 319 7 | -0.528 577 383 791 | -0.525 057 264 58 | -0.521 706 119 2 |
| 47 -0.530 232 139 504 5 | -0.526 620 415 839 | -0.523 177 141 20 | -0.519 903 166 6 |
| 48 -0.528 207 313 545 9 | -0.524 673 120 301 | -0.521 307 558 80 | -0.518 111 770 4 |
| 49 -0.526 192 886 243 2 | -0.522 736 992 180 | -0.519 450 050 49 | -0.516 333 518 6 |
| 50 -0.524 190 291 589 6 | -0.520 813 498 456 | -0.517 606 131 04 | -0.514 569 993 2 |
| 51 -0.522 200 931 870 4 | -0.518 904 083 055 | -0.515 777 303 23 | -0.512 822 778 9 |
| 52 -0.520 226 182 104 3 | -0.517 010 172 357 | -0.513 965 064 96 | -0.511 093 472 8 |
| 53 -0.518 267 394 886 3 | -0.515 133 181 376 | -0.512 170 917 53 | -0.509 383 695 9 |
| 54 -0.516 325 905 713 6 | -0.513 274 520 748 | -0.510 396 375 32 | -0.507 695 107 0 |
| 55 -0.514 403 038 899 0 | -0.511 435 604 758 | -0.508 642 977 24 | -0.506 029 420 6 |
| 56 -0.512 500 114 211 8 | -0.509 617 860 665 | -0.506 912 300 64 | -0.504 388 428 3 |
| 57 -0.510 618 454 433 7 | -0.507 822 739 742 | -0.505 205 978 29 | -0.502 774 027 1 |
| 58 -0.508 759 394 080 4 | -0.506 051 730 550 | -0.503 525 719 95 | -0.501 188 256 2 |
| 59 -0.506 924 289 631 3 | -0.504 306 375 245 | -0.501 873 339 99 | -0.499 633 348 3 |
| 60 -0.505 114 531 741 2 | -0.502 588 290 012 | -0.500 250 794 05 | -0.498 111 800 5 |
| 61 -0.503 331 560 100 5 | -0.500 899 191 343 | -0.498 660 229 06 | -0.496 626 48 |
| 62 -0.501 576 881 907 7 | -0.499 240 930 722 | -0.497 104 054 16 | -0.495 180 78 |
| 63 -0.499 852 095 376 7 | -0.497 615 541 903 | -0.495 585 045 64 | -0.493 778 9 |
| 64 -0.498 158 920 453 2 | -0.496 025 307 747 | -0.494 106 511 | -0.492 426 |
| 65 -0.496 499 240 184 4 | -0.494 472 859 0 | -0.492 672 5 | -0.491 13 |
| 66 -0.494 875 158 447 9 | -0.492 961 329 | -0.491 288 | |
| 67 -0.493 289 084 03 | -0.491 494 6 | | |
| 68 -0.491 743 86 | | | |

Quadrupole transitions per time unit are easily obtained using the wave functions ob-

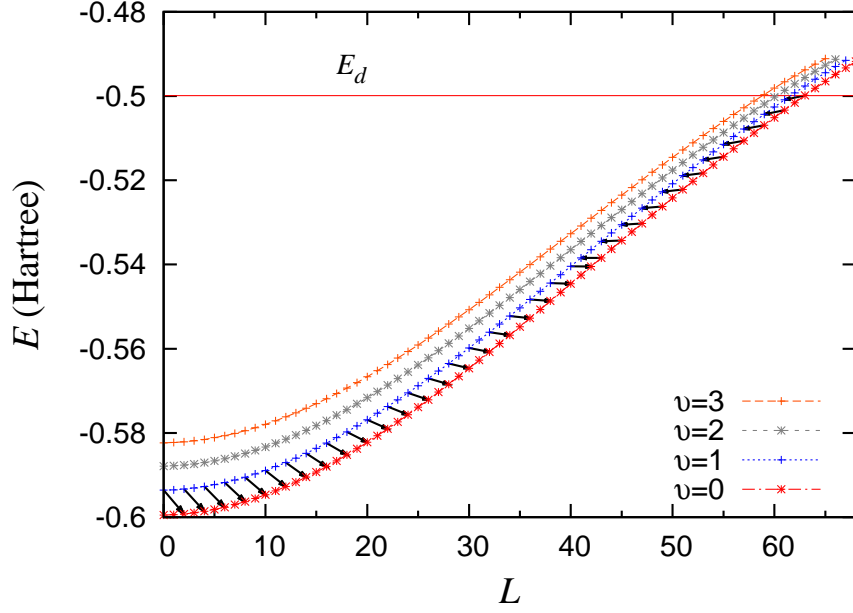


FIG. 1. Four lowest Σ_g rotational bands of the T_2^+ molecular ion and dissociation energy E_d . Arrows show how the direction of $L \rightarrow L + 2$ transitions between the two lowest bands changes along the band.

tained with the Lagrange-mesh method. Table II presents all the probabilities per second for transitions within the same rotational band, $L_f = L_i - 2$ and $v_f = v_i \leq 3$. Some transition probabilities involving quasibound states are presented and these are separated by a horizontal bar. The probabilities increase slowly with L reaching a maximum at $L = 55, 53, 52$ and 50 for $v = 0, 1, 2$ and 3 , respectively.

TABLE II: Quadrupole transition probabilities per second W for transitions between states of a same rotational band ($v_f = v_i$, $L_f = L_i - 2$). Results are given with five digits followed by the power of 10.

| L_i | $v_i = 0$ | $v_i = 1$ | $v_i = 2$ | $v_i = 3$ |
|-------|-------------|-------------|-------------|-------------|
| 2 | 4.077 29-14 | 4.087 46-14 | 4.069 14-14 | 4.024 12-14 |
| 3 | 6.703 22-13 | 6.717 68-13 | 6.685 44-13 | 6.609 46-13 |
| 4 | 3.971 67-12 | 3.978 26-12 | 3.957 28-12 | 3.910 52-12 |

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TABLE II – Continuation

| L_i | $v_i = 0$ | $v_i = 1$ | $v_i = 2$ | $v_i = 3$ |
|-------|-------------|-------------|-------------|-------------|
| 5 | 1.463 26-11 | 1.464 72-11 | 1.456 08-11 | 1.438 00-11 |
| 6 | 4.086 27-11 | 4.086 99-11 | 4.059 72-11 | 4.006 31-11 |
| 7 | 9.510 01-11 | 9.502 44-11 | 9.430 29-11 | 9.297 96-11 |
| 8 | 1.944 69-10 | 1.940 97-10 | 1.924 18-10 | 1.895 23-10 |
| 9 | 3.609 63-10 | 3.598 19-10 | 3.562 77-10 | 3.505 11-10 |
| 10 | 6.213 50-10 | 6.185 18-10 | 6.116 15-10 | 6.009 44-10 |
| 11 | 1.006 81-09 | 1.000 69-09 | 9.880 86-10 | 9.694 84-10 |
| 12 | 1.552 29-09 | 1.540 34-09 | 1.518 55-09 | 1.487 70-09 |
| 13 | 2.295 73-09 | 2.274 07-09 | 2.238 13-09 | 2.189 10-09 |
| 14 | 3.277 02-09 | 3.240 08-09 | 3.183 20-09 | 3.108 09-09 |
| 15 | 4.536 88-09 | 4.477 00-09 | 4.390 15-09 | 4.278 75-09 |
| 16 | 6.115 72-09 | 6.022 70-09 | 5.894 26-09 | 5.733 72-09 |
| 17 | 8.052 40-09 | 7.913 12-09 | 7.728 51-09 | 7.503 01-09 |
| 18 | 1.038 31-08 | 1.018 11-08 | 9.922 49-09 | 9.612 99-09 |
| 19 | 1.314 02-08 | 1.285 55-08 | 1.250 14-08 | 1.208 55-08 |
| 20 | 1.635 14-08 | 1.595 99-08 | 1.548 53-08 | 1.493 69-08 |
| 21 | 2.003 87-08 | 1.951 24-08 | 1.888 83-08 | 1.817 78-08 |
| 22 | 2.421 80-08 | 2.352 47-08 | 2.271 81-08 | 2.181 23-08 |
| 23 | 2.889 84-08 | 2.800 16-08 | 2.697 59-08 | 2.583 81-08 |
| 24 | 3.408 19-08 | 3.294 11-08 | 3.165 59-08 | 3.024 62-08 |
| 25 | 3.976 35-08 | 3.833 42-08 | 3.674 57-08 | 3.502 11-08 |
| 26 | 4.593 08-08 | 4.416 49-08 | 4.222 61-08 | 4.014 11-08 |
| 27 | 5.256 45-08 | 5.041 08-08 | 4.807 19-08 | 4.557 85-08 |
| 28 | 5.963 87-08 | 5.704 28-08 | 5.425 20-08 | 5.130 06-08 |
| 29 | 6.712 11-08 | 6.402 66-08 | 6.072 98-08 | 5.726 95-08 |
| 30 | 7.497 37-08 | 7.132 21-08 | 6.746 44-08 | 6.344 33-08 |
| 31 | 8.315 34-08 | 7.888 51-08 | 7.441 05-08 | 6.977 67-08 |

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TABLE II – Continuation

| L_i | $v_i = 0$ | $v_i = 1$ | $v_i = 2$ | $v_i = 3$ |
|-------|-------------|-------------|-------------|-------------|
| 32 | 9.161 25-08 | 8.666 71-08 | 8.151 96-08 | 7.622 13-08 |
| 33 | 1.002 99-07 | 9.461 67-08 | 8.874 06-08 | 8.272 68-08 |
| 34 | 1.091 60-07 | 1.026 80-07 | 9.602 01-08 | 8.924 12-08 |
| 35 | 1.181 37-07 | 1.108 00-07 | 1.033 04-07 | 9.571 18-08 |
| 36 | 1.271 71-07 | 1.189 20-07 | 1.105 36-07 | 1.020 85-07 |
| 37 | 1.362 03-07 | 1.269 83-07 | 1.176 62-07 | 1.083 10-07 |
| 38 | 1.451 72-07 | 1.349 31-07 | 1.246 26-07 | 1.143 32-07 |
| 39 | 1.540 19-07 | 1.427 07-07 | 1.313 75-07 | 1.201 02-07 |
| 40 | 1.626 84-07 | 1.502 54-07 | 1.378 55-07 | 1.255 71-07 |
| 41 | 1.711 09-07 | 1.575 18-07 | 1.440 17-07 | 1.306 91-07 |
| 42 | 1.792 38-07 | 1.644 46-07 | 1.498 11-07 | 1.354 19-07 |
| 43 | 1.870 16-07 | 1.709 89-07 | 1.551 90-07 | 1.397 11-07 |
| 44 | 1.943 90-07 | 1.770 97-07 | 1.601 12-07 | 1.435 28-07 |
| 45 | 2.013 13-07 | 1.827 27-07 | 1.645 36-07 | 1.468 33-07 |
| 46 | 2.077 36-07 | 1.878 36-07 | 1.684 22-07 | 1.495 92-07 |
| 47 | 2.136 18-07 | 1.923 84-07 | 1.717 37-07 | 1.517 76-07 |
| 48 | 2.189 17-07 | 1.963 36-07 | 1.744 48-07 | 1.533 55-07 |
| 49 | 2.235 97-07 | 1.996 58-07 | 1.765 27-07 | 1.543 04-07 |
| 50 | 2.276 23-07 | 2.023 22-07 | 1.779 47-07 | 1.546 02-07 |
| 51 | 2.309 67-07 | 2.042 99-07 | 1.786 85-07 | 1.542 28-07 |
| 52 | 2.336 01-07 | 2.055 68-07 | 1.787 20-07 | 1.531 66-07 |
| 53 | 2.355 00-07 | 2.061 05-07 | 1.780 35-07 | 1.513 99-07 |
| 54 | 2.366 45-07 | 2.058 95-07 | 1.766 13-07 | 1.489 14-07 |
| 55 | 2.370 16-07 | 2.049 19-07 | 1.744 41-07 | 1.456 98-07 |
| 56 | 2.366 00-07 | 2.031 65-07 | 1.715 05-07 | 1.417 41-07 |
| 57 | 2.353 84-07 | 2.006 20-07 | 1.677 93-07 | 1.370 29-07 |
| 58 | 2.333 55-07 | 1.972 73-07 | 1.632 94-07 | 1.315 50-07 |

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TABLE II – Continuation

| L_i | $v_i = 0$ | $v_i = 1$ | $v_i = 2$ | $v_i = 3$ |
|-------|-------------|-------------|-------------|-------------|
| 59 | 2.305 07-07 | 1.931 13-07 | 1.579 94-07 | 1.252 87-07 |
| 60 | 2.268 30-07 | 1.881 30-07 | 1.518 77-07 | 1.182 18-07 |
| 61 | 2.223 19-07 | 1.823 10-07 | 1.449 24-07 | 1.103 12-07 |
| 62 | 2.169 64-07 | 1.756 37-07 | 1.371 06-07 | 1.015 22-07 |
| 63 | 2.107 59-07 | 1.680 90-07 | 1.283 81-07 | 9.177 09-08 |
| 64 | 2.036 91-07 | 1.596 37-07 | 1.186 85-07 | 8.093 00-08 |
| 65 | 1.957 44-07 | 1.502 31-07 | 1.079 16-07 | 6.874 67-08 |
| 66 | 1.868 92-07 | 1.397 98-07 | 9.589 20-08 | |
| 67 | 1.770 96-07 | 1.282 13-07 | | |
| 68 | 1.662 90-07 | | | |

Quadrupole transitions per time unit for other transitions are presented in Table III. The columns correspond to transitions between different vibrational states. For each L_i value, the successive lines correspond to increasing values of L_f , i.e. to $L_f = L_i - 2$ for $L_i > 1$, $L_f = L_i$ for $L_i > 0$, and $L_f = L_i + 2$, respectively. The strongest transition from each state occurs in general towards the nearest vibrational state ($v_f = v_i - 1$) for $L_f = L_i - 2$. For $v_f = v_i - 1$, in the vicinity of $L_i = 41$, and beyond, the $(L_i, v_i) \rightarrow (L_i + 2, v_i - 1)$ transitions are replaced by $(L_i + 2, v_i - 1) \rightarrow (L_i, v_i)$ transitions because the sign of the energy difference changes (see the arrows in Figure 1 for the 10 transitions). These numbers are indicated in italics in Table III. For example, the first number in the last line for $L_i = 41$ corresponds to the $(43, 0) \rightarrow (41, 1)$ transition. Hence, the transition probabilities strongly vary in this region.

TABLE III: Quadrupole transition probabilities per second W for transitions between different vibrational quantum numbers ($v_i \neq v_f$). The three successive lines correspond to increasing L_f values, i.e. $L_f = L_i - 2$, $L_f = L_i$ and $L_f = L_i + 2$, respectively, for $L_i \geq 2$. Italicized numbers for $(1 \rightarrow 0)$, $(2 \rightarrow 1)$ and $(3 \rightarrow 2)$ mean that the initial and final states are exchanged (the first one is preceded in each case by a horizontal bar).

| L_i | $(1 \rightarrow 0)$ | $(2 \rightarrow 0)$ | $(2 \rightarrow 1)$ | $(3 \rightarrow 0)$ | $(3 \rightarrow 1)$ | $(3 \rightarrow 2)$ |
|-------|---------------------|---------------------|---------------------|---------------------|---------------------|---------------------|
| 0 | 2.352 92−08 | 1.966 46−09 | 4.209 56−08 | 1.218 32−10 | 5.449 55−09 | 5.631 51−08 |
| 1 | 1.076 05−08 | 1.025 38−09 | 1.920 69−08 | 7.676 43−11 | 2.817 57−09 | 2.563 57−08 |
| | 1.278 01−08 | 9.691 38−10 | 2.289 40−08 | 5.114 59−11 | 2.702 85−09 | 3.066 63−08 |
| 2 | 6.053 60−09 | 6.477 38−10 | 1.077 63−08 | 5.616 33−11 | 1.766 56−09 | 1.434 44−08 |
| | 7.668 00−09 | 7.318 48−10 | 1.368 58−08 | 5.487 71−11 | 2.010 80−09 | 1.826 48−08 |
| | 9.839 31−09 | 6.702 09−10 | 1.764 53−08 | 2.889 74−11 | 1.882 55−09 | 2.366 10−08 |
| 3 | 8.334 47−09 | 9.577 09−10 | 1.480 60−08 | 9.016 18−11 | 2.599 81−09 | 1.966 74−08 |
| | 7.131 55−09 | 6.822 58−10 | 1.272 66−08 | 5.128 11−11 | 1.874 29−09 | 1.698 23−08 |
| | 8.118 99−09 | 4.906 61−10 | 1.457 34−08 | 1.621 87−11 | 1.389 52−09 | 1.955 89−08 |
| 4 | 9.839 96−09 | 1.209 31−09 | 1.744 09−08 | 1.224 32−10 | 3.268 27−09 | 2.311 43−08 |
| | 6.913 64−09 | 6.634 88−10 | 1.233 56−08 | 5.002 82−11 | 1.822 39−09 | 1.645 73−08 |
| | 6.852 13−09 | 3.618 13−10 | 1.230 83−08 | 8.249 22−12 | 1.034 47−09 | 1.653 02−08 |
| 5 | 1.100 38−08 | 1.441 38−09 | 1.945 56−08 | 1.557 27−10 | 3.878 88−09 | 2.571 96−08 |
| | 6.784 85−09 | 6.536 72−10 | 1.210 31−08 | 4.948 10−11 | 1.795 02−09 | 1.614 33−08 |
| | 5.825 36−09 | 2.636 09−10 | 1.046 95−08 | 3.389 76−12 | 7.623 79−10 | 1.406 77−08 |
| 6 | 1.195 55−08 | 1.664 33−09 | 2.108 16−08 | 1.906 95−10 | 4.460 38−09 | 2.779 29−08 |
| | 6.687 94−09 | 6.473 36−10 | 1.192 71−08 | 4.922 88−11 | 1.777 14−09 | 1.590 39−08 |
| | 4.956 19−09 | 1.874 69−10 | 8.910 54−09 | 8.223 10−13 | 5.499 08−10 | 1.197 65−08 |
| 7 | 1.274 29−08 | 1.880 78−09 | 2.240 48−08 | 2.273 62−10 | 5.020 13−09 | 2.944 95−08 |
| | 6.602 78−09 | 6.425 42−10 | 1.177 15−08 | 4.912 48−11 | 1.763 42−09 | 1.569 13−08 |

Continued on Next Page...

TABLE III – Continuation

| L_i | $(1 \rightarrow 0)$ | $(2 \rightarrow 0)$ | $(2 \rightarrow 1)$ | $(3 \rightarrow 0)$ | $(3 \rightarrow 1)$ | $(3 \rightarrow 2)$ |
|-------|---------------------|---------------------|---------------------|---------------------|---------------------|---------------------|
| | 4.205 83–09 | 1.286 50–10 | 7.562 74–09 | 3.163–15 | 3.842 83–10 | 1.016 60–08 |
| 8 | 1.338 44–08 | 2.090 35–09 | 2.345 90–08 | 2.654 77–10 | 5.557 41–09 | 3.073 59–08 |
| | 6.520 84–09 | 6.384 48–10 | 1.162 13–08 | 4.910 45–11 | 1.751 56–09 | 1.548 51–08 |
| | 3.553 06–09 | 8.398 43–11 | 6.388 81–09 | 5.151 4 –13 | 2.570 35–10 | 8.587 19–09 |
| 9 | 1.388 65–08 | 2.291 35–09 | 2.425 70–08 | 3.046 33–10 | 6.067 94–09 | 3.167 10–08 |
| | 6.438 02–09 | 6.346 37–10 | 1.146 91–08 | 4.913 45–11 | 1.740 42–09 | 1.527 57–08 |
| | 2.984 49–09 | 5.105 00–11 | 5.365 33–09 | 2.015 57–12 | 1.617 32–10 | 7.209 46–09 |
| 10 | 1.425 08–08 | 2.481 48–09 | 2.480 33–08 | 3.443 26–10 | 6.545 88–09 | 3.226 30–08 |
| | 6.352 26–09 | 6.308 78–10 | 1.131 13–08 | 4.919 57–11 | 1.729 36–09 | 1.505 82–08 |
| | 2.490 52–09 | 2.784 36–11 | 4.475 49–09 | 4.215 75–12 | 9.305 25–11 | 6.010 82–09 |
| 11 | 1.447 76–08 | 2.658 16–09 | 2.510 01–08 | 3.839 88–10 | 6.984 74–09 | 3.251 72–08 |
| | 6.262 43–09 | 6.270 34–10 | 1.114 59–08 | 4.927 55–11 | 1.718 00–09 | 1.483 01–08 |
| | 2.063 39–09 | 1.263 30–11 | 3.705 70–09 | 6.871 68–12 | 4.639 12–11 | 4.973 47–09 |
| 12 | 1.456 72–08 | 2.818 84–09 | 2.515 01–08 | 4.230 17–10 | 7.378 14–09 | 3.244 01–08 |
| | 6.167 98–09 | 6.230 15–10 | 1.097 19–08 | 4.936 50–11 | 1.706 11–09 | 1.459 01–08 |
| | 1.696 33–09 | 3.893 88–12 | 3.044 04–09 | 9.779 27–12 | 1.768 15–11 | 4.081 72–09 |
| 13 | 1.452 14–08 | 2.961 08–09 | 2.495 86–08 | 4.608 01–10 | 7.720 13–09 | 3.204 18–08 |
| | 6.068 67–09 | 6.187 63–10 | 1.078 89–08 | 4.945 75–11 | 1.693 54–09 | 1.433 77–08 |
| | 1.383 15–09 | 2.803 80–13 | 2.479 52–09 | 1.277 08–11 | 3.317 84–12 | 3.320 98–09 |
| 14 | 1.434 34–08 | 3.082 73–09 | 2.453 38–08 | 4.967 37–10 | 8.005 53–09 | 3.133 67–08 |
| | 5.964 42–09 | 6.142 34–10 | 1.059 69–08 | 4.954 74–11 | 1.680 16–09 | 1.407 28–08 |
| | 1.118 03–09 | 6.106 10–13 | 2.001 77–09 | 1.571 20–11 | 1.196 23–13 | 2.677 42–09 |
| 15 | 1.403 87–08 | 3.181 97–09 | 2.388 79–08 | 5.302 5–10 | 8.230 1–09 | 3.034 38–08 |
| | 5.855 30–09 | 6.093 99–10 | 1.039 60–08 | 4.963 01–11 | 1.665 90–09 | 1.379 58–08 |
| | 8.954 75–10 | 3.857 94–12 | 1.600 94–09 | 1.849 87–11 | 5.310 1–12 | 2.137 81–09 |
| 16 | 1.361 45–08 | 3.257 39–09 | 2.303 62–08 | 5.608 17–10 | 8.390 8–09 | 2.908 72–08 |
| | 5.741 47–09 | 6.042 34–10 | 1.018 65–08 | 4.970 17–11 | 1.650 69–09 | 1.350 70–08 |

Continued on Next Page...

TABLE III – Continuation

| L_i ($1 \rightarrow 0$) | ($2 \rightarrow 0$) | ($2 \rightarrow 1$) | ($3 \rightarrow 0$) | ($3 \rightarrow 1$) | ($3 \rightarrow 2$) | |
|-----------------------------|-----------------------|-----------------------|-----------------------|-----------------------|-----------------------|-------------|
| | 7.103 10–10 | 9.143 31–12 | 1.267 71–09 | 2.105 36–11 | 1.649 90–11 | 1.689 62–09 |
| 17 | 1.308 04–08 | 3.308 04–09 | 2.199 77–08 | 5.879 7–10 | 8.485 83–09 | 2.759 50–08 |
| | 5.623 14–09 | 5.987 25–10 | 9.968 78–09 | 4.975 87–11 | 1.634 51–09 | 1.320 71–08 |
| | 5.576 85–10 | 1.572 69–11 | 9.933 25–10 | 2.332 30–11 | 3.166 31–11 | 1.321 02–09 |
| 18 | 1.244 73–08 | 3.333 43–09 | 2.079 44–08 | 6.113 1–10 | 8.514 4–09 | 2.589 92–08 |
| | 5.500 56–09 | 5.928 59–10 | 9.743 38–09 | 4.979 82–11 | 1.617 32–09 | 1.289 68–08 |
| | 4.331 11–10 | 2.299 86–11 | 7.696 66–10 | 2.527 31–11 | 4.912 29–11 | 1.021 00–09 |
| 19 | 1.172 80–08 | 3.333 5–09 | 1.945 07–08 | 6.305 3–10 | 8.477 1–09 | 2.403 50–08 |
| | 5.374 02–09 | 5.866 29–10 | 9.510 84–09 | 4.981 75–11 | 1.599 11–09 | 1.257 68–08 |
| | 3.324 75–10 | 3.046 69–11 | 5.892 76–10 | 2.688 68–11 | 6.751 52–11 | 7.794 50–10 |
| 20 | 1.093 63–08 | 3.308 75–09 | 1.799 29–08 | 6.453 9–10 | 8.375 8–09 | 2.203 97–08 |
| | 5.243 83–09 | 5.800 32–10 | 9.271 75–09 | 4.981 44–11 | 1.579 86–09 | 1.224 81–08 |
| | 2.520 58–10 | 3.774 70–11 | 4.454 05–10 | 2.816 09–11 | 8.576 37–11 | 5.872 12–10 |
| 21 | 1.008 72–08 | 3.259 9–09 | 1.644 9–08 | 6.557 60–10 | 8.213 3–09 | 1.995 20–08 |
| | 5.110 33–09 | 5.730 67–10 | 9.026 73–09 | 4.978 72–11 | 1.559 59–09 | 1.191 14–08 |
| | 1.885 36–10 | 4.454 87–11 | 3.320 16–10 | 2.910 27–11 | 1.030 46–10 | 4.360 81–10 |
| 22 | 9.196 0–09 | 3.188 4–09 | 1.484 74–08 | 6.615 5–10 | 7.993 4–09 | 1.781 11–08 |
| | 4.973 86–09 | 5.657 36–10 | 8.776 43–09 | 4.973 42–11 | 1.538 29–09 | 1.156 77–08 |
| | 1.389 74–10 | 5.066 35–11 | 2.437 80–10 | 2.972 75–11 | 1.187 62–10 | 3.188 17–10 |
| 23 | 8.278 55–09 | 3.095 7–09 | 1.321 70–08 | 6.628 1–10 | 7.720 7–09 | 1.565 62–08 |
| | 4.834 76–09 | 5.580 44–10 | 8.521 50–09 | 4.965 44–11 | 1.515 99–09 | 1.121 79–08 |
| | 1.008 13–10 | 5.595 26–11 | 1.760 51–10 | 3.005 69–11 | 1.325 01–10 | 2.291 12–10 |
| 24 | 7.350 4–09 | 2.983 6–09 | 1.158 6–08 | 6.596 1–10 | 7.400 6–09 | 1.352 5–08 |
| | 4.693 41–09 | 5.499 98–10 | 8.262 61–09 | 4.954 69–11 | 1.492 71–09 | 1.086 30–08 |
| | 7.185 10–11 | 6.033 52–11 | 1.248 31–10 | 3.011 60–11 | 1.440 11–10 | 1.615 38–10 |
| 25 | 6.427 0–09 | 2.854 39–09 | 9.981 4–09 | 6.521 4–10 | 7.038 9–09 | 1.145 4–08 |
| | 4.550 15–09 | 5.416 06–10 | 8.000 44–09 | 4.941 11–11 | 1.468 46–09 | 1.050 38–08 |

Continued on Next Page...

TABLE III – Continuation

| L_i | (1 \rightarrow 0) | (2 \rightarrow 0) | (2 \rightarrow 1) | (3 \rightarrow 0) | (3 \rightarrow 1) | (3 \rightarrow 2) |
|-------|---------------------|---------------------|---------------------|---------------------|---------------------|---------------------|
| | 5.021 28–11 | 6.377 79–11 | 8.672 25–11 | 2.993 26–11 | 1.531 71–10 | 1.114 92–10 |
| 26 | 5.523 16–09 | 2.710 2–09 | 8.429 80–09 | 6.406 0–10 | 6.641 95–09 | 9.477 97–09 |
| | 4.405 34–09 | 5.328 79–10 | 7.735 64–09 | 4.924 68–11 | 1.443 29–09 | 1.014 14–08 |
| | 3.432 55–11 | 6.628 48–11 | 5.887 73–11 | 2.953 53–11 | 1.599 65–10 | 7.512 05–11 |
| 27 | 4.652 76–09 | 2.553 44–09 | 6.955 2–09 | 6.252 7–10 | 6.216 2–09 | 7.627 4–09 |
| | 4.259 35–09 | 5.238 29–10 | 7.468 89–09 | 4.905 39–11 | 1.417 23–09 | 9.776 61–09 |
| | 2.288 51–11 | 6.788 90–11 | 3.893 97–11 | 2.895 29–11 | 1.644 55–10 | 4.924 11–11 |
| 28 | 3.828 79–09 | 2.386 6–09 | 5.579 9–09 | 6.064 9–10 | 5.768 3–09 | 5.930 9–09 |
| | 4.112 52–09 | 5.144 70–10 | 7.200 83–09 | 4.883 29–11 | 1.390 30–09 | 9.410 36–09 |
| | 1.482 59–11 | 6.864 49–11 | 2.498 85–11 | 2.821 34–11 | 1.667 68–10 | 3.126 69–11 |
| 29 | 3.063 0–09 | 2.212 26–09 | 4.323 80–09 | 5.845 8–10 | 5.304 95–09 | 4.413 36–09 |
| | 3.965 19–09 | 5.048 16–10 | 6.932 10–09 | 4.858 40–11 | 1.362 57–09 | 9.043 54–09 |
| | 9.289 68–12 | 6.862 23–11 | 1.548 11–11 | 2.734 34–11 | 1.670 72–10 | 1.912 68–11 |
| 30 | 2.365 97–09 | 2.032 79–09 | 3.204 24–09 | 5.599 29–10 | 4.832 60–09 | 3.096 05–09 |
| | 3.817 71–09 | 4.948 82–10 | 6.663 32–09 | 4.830 79–11 | 1.334 06–09 | 8.677 02–09 |
| | 5.596 29–12 | 6.790 03–11 | 9.199 19–12 | 2.636 76–11 | 1.655 62–10 | 1.119 16–11 |
| 31 | 1.746 77–09 | 1.850 63–09 | 2.236 07–09 | 5.329 18–10 | 4.357 58–09 | 1.996 57–09 |
| | 3.670 39–09 | 4.846 86–10 | 6.395 09–09 | 4.800 55–11 | 1.304 83–09 | 8.311 61–09 |
| | 3.216 00–12 | 6.656 34–11 | 5.198 05–12 | 2.530 91–11 | 1.624 53–10 | 6.204 20–12 |
| 32 | 1.213 15–09 | 1.668 10–09 | 1.431 46–09 | 5.039 43–10 | 3.885 89–09 | 1.128 80–09 |
| | 3.523 55–09 | 4.742 43–10 | 6.127 98–09 | 4.767 77–11 | 1.274 92–09 | 7.948 14–09 |
| | 1.744 50–12 | 6.469 81–11 | 2.760 53–12 | 2.418 85–11 | 1.579 65–10 | 3.216 05–12 |
| 33 | 7.714 1–10 | 1.487 39–09 | 7.999 1–10 | 4.733 98–10 | 3.423 18–09 | 5.029 3–10 |
| | 3.377 49–09 | 4.635 71–10 | 5.862 57–09 | 4.732 57–11 | 1.244 37–09 | 7.587 36–09 |
| | 8.802 65–13 | 6.238 95–11 | 1.355 38–12 | 2.302 43–11 | 1.523 18–10 | 1.529 98–12 |
| 34 | 4.264 6–10 | 1.310 55–09 | 3.483 6–10 | 4.416 7–10 | 2.974 70–09 | 1.255 9–10 |
| | 3.232 50–09 | 4.526 88–10 | 5.599 37–09 | 4.695 05–11 | 1.213 25–09 | 7.230 01–09 |

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TABLE III – Continuation

| L_i | $(1 \rightarrow 0)$ | $(2 \rightarrow 0)$ | $(2 \rightarrow 1)$ | $(3 \rightarrow 0)$ | $(3 \rightarrow 1)$ | $(3 \rightarrow 2)$ |
|-------|---------------------|---------------------|---------------------|---------------------|---------------------|---------------------|
| | 4.045 46–13 | 5.971 99–11 | 6.005 87–13 | 2.183 29–11 | 1.457 23–10 | 6.496 11–13 |
| 35 | 1.817 9–10 | 1.139 50–09 | 8.119–11 | 4.091 4–10 | 2.545 26–09 | 5.494–16 |
| | 3.088 87–09 | 4.416 10–10 | 5.338 90–09 | 4.655 34–11 | 1.181 59–09 | 6.876 79–09 |
| | 1.639 80–13 | 5.676 68–11 | 2.313 56–13 | 2.062 86–11 | 1.383 84–10 | 2.354 82–13 |
| 36 | 3.960 1–11 | 9.759 5–10 | 4.209–13 | 3.761 56–10 | 2.139 20–09 | 1.261 19–10 |
| | 2.946 83–09 | 4.303 56–10 | 5.081 64–09 | 4.613 58–11 | 1.149 44–09 | 6.528 36–09 |
| | 5.563 95–14 | 5.360 21–11 | 7.277 03–14 | 1.942 37–11 | 1.304 86–10 | 6.748 60–14 |
| 37 | 8.078–13 | 8.214 7–10 | 1.058 0–10 | 3.430 7–10 | 1.760 4–09 | 5.009 0–10 |
| | 2.806 65–09 | 4.189 43–10 | 4.828 03–09 | 4.569 88–11 | 1.116 85–09 | 6.185 35–09 |
| | 1.438 79–14 | 5.029 16–11 | 1.661 93–14 | 1.822 85–11 | 1.222 03–10 | 1.313 86–14 |
| 38 | 6.516–11 | 6.774 36–10 | 3.950 1–10 | 3.102 08–10 | 1.412 30–09 | 1.118 53–09 |
| | 2.668 56–09 | 4.073 87–10 | 4.578 50–09 | 4.524 39–11 | 1.083 87–09 | 5.848 33–09 |
| | 2.331 32–15 | 4.689 41–11 | 2.118 82–15 | 1.705 19–11 | 1.136 88–10 | 1.197 40–15 |
| 39 | 2.313 39–10 | 5.450 6–10 | 8.637 9–10 | 2.778 6–10 | 1.097 81–09 | 1.970 66–09 |
| | 2.532 76–09 | 3.957 06–10 | 4.333 45–09 | 4.477 23–11 | 1.050 54–09 | 5.517 86–09 |
| | 1.386 40–16 | 4.346 17–11 | 6.554 54–17 | 1.590 12–11 | 1.050 80–10 | 1.160 54–17 |
| 40 | 4.970 1–10 | 4.253 9–10 | 1.506 18–09 | 2.463 07–10 | 8.194 6–10 | 3.046 6–09 |
| | 2.399 47–09 | 3.839 15–10 | 4.093 24–09 | 4.428 52–11 | 1.016 91–09 | 5.194 44–09 |
| | 1.484 82–19 | 4.004 02–11 | 2.290 73–26 | 1.478 21–11 | 9.649 65–11 | <i>3.553 47–19</i> |
| 41 | 8.589 7–10 | 3.193 17–10 | 2.314 67–09 | 2.158 00–10 | 5.793 48–10 | 4.333 86–09 |
| | <u>2.268 86–09</u> | <u>3.720 31–10</u> | <u>3.858 22–09</u> | 4.378 38–11 | 9.830 22–10 | 4.878 53–09 |
| | <i>3.300 74–18</i> | 3.666 84–11 | <i>5.047 82–17</i> | 1.369 94–11 | 8.804 22–11 | <i>3.384 62–16</i> |
| 42 | 1.313 23–09 | 2.275 68–10 | 3.280 37–09 | 1.865 7–10 | 3.791 8–10 | 5.817 89–09 |
| | 2.141 12–09 | 3.600 68–10 | 3.628 71–09 | 4.326 93–11 | 9.489 15–10 | 4.570 56–09 |
| | <i>3.274 43–16</i> | 3.337 97–11 | <i>1.605 87–15</i> | 1.265 68–11 | 7.980 38–11 | <i>5.325 31–15</i> |
| 43 | 1.855 11–09 | 1.507 49–10 | 4.393 24–09 | 1.588 36–10 | 2.203 26–10 | 7.482 77–09 |
| | 2.016 39–09 | 3.480 41–10 | 3.404 97–09 | 4.274 27–11 | 9.146 32–10 | 4.270 93–09 |

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TABLE III – Continuation

| L_i ($1 \rightarrow 0$) | ($2 \rightarrow 0$) | ($2 \rightarrow 1$) | ($3 \rightarrow 0$) | ($3 \rightarrow 1$) | ($3 \rightarrow 2$) |
|-----------------------------|-----------------------|-----------------------|-----------------------|-----------------------|-----------------------|
| <i>3.346 80–15</i> | 3.020 12–11 | <i>1.187 03–14</i> | 1.165 67–11 | 7.185 34–11 | <i>3.049 73–14</i> |
| 44 2.479 36–09 | 8.933 87–11 | 5.642 2–09 | 1.327 8–10 | 1.038 2–10 | 9.311 25–09 |
| | 1.894 81–09 | 3.359 63–10 | 3.187 29–09 | 4.220 48–11 | 8.802 10–10 |
| | 3.980 00–09 | | | | |
| <i>1.592 91–14</i> | 2.715 53–11 | <i>4.847 99–14</i> | 1.070 13–11 | 6.424 96–11 | <i>1.092 26–13</i> |
| 45 3.180 20–09 | 4.370 6–11 | 7.015 36–09 | 1.085 86–10 | 3.043–11 | 1.128 50–08 |
| | 1.776 53–09 | 3.238 48–10 | 2.975 88–09 | 4.165 65–11 | 8.456 87–10 |
| | 3.698 07–09 | | | | |
| <i>5.143 45–14</i> | 2.425 93–11 | <i>1.432 61–13</i> | 9.791 66–12 | 5.703 82–11 | <i>2.980 88–13</i> |
| 46 3.951 50–09 | 1.412 8–11 | 8.500 1–09 | 8.641 2–11 | 6.898–13 | 1.338 4–08 |
| | 1.661 64–09 | 3.117 09–10 | 2.770 96–09 | 4.109 84–11 | 8.110 97–10 |
| | 3.425 44–09 | | | | |
| <i>1.313 00–13</i> | 2.152 65–11 | <i>3.453 00–13</i> | 8.928 43–12 | 5.025 38–11 | <i>6.814 32–13</i> |
| 47 4.786 76–09 | 8.061–13 | 1.008 33–08 | 6.641 4–11 | 1.493 2–11 | 1.559 01–08 |
| | 1.550 27–09 | 2.995 57–10 | 2.572 72–09 | 4.053 08–11 | 7.764 74–10 |
| | 3.162 36–09 | | | | |
| <i>2.863 53–13</i> | 1.896 63–11 | <i>7.236 25–13</i> | 8.111 81–12 | 4.392 10–11 | <i>1.375 59–12</i> |
| 48 5.679 28–09 | 3.879 6–12 | 1.175 13–08 | 4.873 7–11 | 7.334 1–11 | 1.788 08–08 |
| | 1.442 48–09 | 2.874 03–10 | 2.381 32–09 | 3.995 41–11 | 7.418 49–10 |
| | 2.909 04–09 | | | | |
| <i>5.580 06–13</i> | 1.658 46–11 | <i>1.369 78–12</i> | 7.341 58–12 | 3.805 53–11 | <i>2.533 21–12</i> |
| 49 6.622 16–09 | 2.344 7–11 | 1.349 02–08 | 3.352 95–11 | 1.759 97–10 | 2.023 55–08 |
| | 1.338 38–09 | 2.752 57–10 | 2.196 90–09 | 3.936 83–11 | 7.072 52–10 |
| | 2.665 69–09 | | | | |
| <i>9.994 50–13</i> | 1.438 48–11 | <i>2.400 60–12</i> | 6.617 19–12 | 3.266 46–11 | <i>4.348 19–12</i> |
| 50 7.608 4–09 | 5.958–11 | 1.528 6–08 | 2.094–11 | 3.229 1–10 | 2.263 2–08 |
| | 1.238 01–09 | 2.631 31–10 | 2.019 58–09 | 3.877 32–11 | 6.727 13–10 |
| | 2.432 45–09 | | | | |
| <i>1.677 03–12</i> | 1.236 73–11 | <i>3.961 54–12</i> | 5.937 86–12 | 2.775 01–11 | <i>7.061 89–12</i> |
| 51 8.630 9–09 | 1.123 5–10 | 1.712 3–08 | 1.113–11 | 5.140 9–10 | 2.504 97–08 |
| | 1.141 43–09 | 2.510 32–10 | 1.849 46–09 | 3.816 82–11 | 6.382 56–10 |
| | 2.209 47–09 | | | | |
| <i>2.671 95–12</i> | 1.053 07–11 | <i>6.230 94–12</i> | 5.302 60–12 | 2.330 70–11 | <i>1.097 12–11</i> |
| 52 9.682 7–09 | 1.818 6–10 | 1.898 9–08 | 4.278–12 | 7.495 6–10 | 2.746 45–08 |
| | 1.048 70–09 | 2.389 69–10 | 1.686 62–09 | 3.755 27–11 | 6.039 07–10 |
| | 1.996 84–09 | | | | |

Continued on Next Page...

TABLE III – Continuation

| L_i | (1 \rightarrow 0) | (2 \rightarrow 0) | (2 \rightarrow 1) | (3 \rightarrow 0) | (3 \rightarrow 1) | (3 \rightarrow 2) |
|-------|---------------------|---------------------|---------------------|---------------------|---------------------|---------------------|
| | <i>4.082 49–12</i> | 8.871 63–12 | <i>9.425 75–12</i> | 4.710 29–12 | 1.932 59–11 | <i>1.643 99–11</i> |
| 53 | 1.075 67–08 | 2.682 1–10 | 2.086 92–08 | 5.923–13 | 1.029 43–09 | 2.985 41–08 |
| | 9.598 52–10 | 2.269 50–10 | 1.531 12–09 | 3.692 52–11 | 5.696 88–10 | 1.794 65–09 |
| | <i>6.027 05–12</i> | 7.385 21–12 | <i>1.380 93–11</i> | 4.159 68–12 | 1.579 30–11 | <i>2.391 37–11</i> |
| 54 | 1.184 60–08 | 3.716 0–10 | 2.274 72–08 | 3.184–13 | 1.353 9–09 | 3.219 47–08 |
| | 8.749 05–10 | 2.149 82–10 | 1.383 02–09 | 3.628 41–11 | 5.356 22–10 | 1.602 97–09 |
| | <i>8.648 33–12</i> | 6.065 34–12 | <i>1.970 25–11</i> | 3.649 46–12 | 1.269 14–11 | <i>3.394 27–11</i> |
| 55 | 1.294 36–08 | 4.923 0–10 | 2.460 91–08 | 3.757 7–12 | 1.723 58–09 | 3.446 19–08 |
| | 7.938 82–10 | 2.030 72–10 | 1.242 34–09 | 3.562 72–11 | 5.017 25–10 | 1.421 82–09 |
| | <i>1.211 91–11</i> | 4.904 85–12 | <i>2.749 85–11</i> | 3.178 28–12 | 1.000 12–11 | <i>4.721 21–11</i> |
| 56 | 1.404 29–08 | 6.307 32–10 | 2.643 99–08 | 1.128 6–11 | 2.139 01–09 | 3.663 00–08 |
| | 7.167 94–10 | 1.912 25–10 | 1.109 10–09 | 3.495 14–11 | 4.680 16–10 | 1.251 22–09 |
| | <i>1.665 01–11</i> | 3.895 79–12 | <i>3.768 54–11</i> | 2.744 75–12 | 7.700 17–12 | <i>6.458 86–11</i> |
| 57 | 1.513 72–08 | 7.874 6–10 | 2.822 44–08 | 2.337 9–11 | 2.601 26–09 | 3.867 15–08 |
| | 6.436 44–10 | 1.794 46–10 | 9.832 96–10 | 3.425 27–11 | 4.345 05–10 | 1.091 18–09 |
| | <i>2.250 18–11</i> | 3.029 52–12 | <i>5.087 71–11</i> | 2.347 51–12 | 5.764 32–12 | <i>8.718 78–11</i> |
| 58 | 1.622 00–08 | 9.632 6–10 | 2.994 65–08 | 4.064 8–11 | 3.111 74–09 | 4.055 65–08 |
| | 5.744 28–10 | 1.677 39–10 | 8.649 25–10 | 3.352 61–11 | 4.012 03–10 | 9.416 67–10 |
| | <i>3.000 06–11</i> | 2.296 89–12 | <i>6.786 01–11</i> | 1.985 18–12 | 4.167 99–12 | <i>1.164 78–10</i> |
| 59 | 1.728 49–08 | 1.159 21–09 | 3.158 95–08 | 6.389 1–11 | 3.672 30–09 | 4.225 13–08 |
| | 5.091 36–10 | 1.561 06–10 | 7.539 64–10 | 3.276 45–11 | 3.681 10–10 | 8.026 58–10 |
| | <i>3.956 26–11</i> | 1.688 35–12 | <i>8.966 33–11</i> | 1.656 45–12 | 2.884 14–12 | <i>1.544 45–10</i> |
| 60 | 1.832 55–08 | 1.376 72–09 | 3.313 53–08 | 9.415 7–11 | 4.285 26–09 | 4.371 62–08 |
| | 4.477 53–10 | 1.445 49–10 | 6.503 81–10 | 3.195 86–11 | 3.352 19–10 | 6.741 05–10 |
| | <i>5.172 91–11</i> | 1.193 95–12 | <i>1.176 66–10</i> | 1.360 00–12 | 1.884 37–12 | <i>2.038 55–10</i> |
| 61 | 1.933 53–08 | 1.617 65–09 | 3.456 35–08 | 1.328 44–10 | 4.953 30–09 | 4.490 23–08 |
| | 3.902 59–10 | 1.330 65–10 | 5.541 36–10 | 3.109 51–11 | 3.025 06–10 | 5.559 48–10 |

Continued on Next Page...

TABLE III – Continuation

| L_i ($1 \rightarrow 0$) | ($2 \rightarrow 0$) | ($2 \rightarrow 1$) | ($3 \rightarrow 0$) | ($3 \rightarrow 1$) | ($3 \rightarrow 2$) |
|-----------------------------|-----------------------|-----------------------|-----------------------|-----------------------|-----------------------|
| <i>6.722 11–11</i> | 8.034 38–13 | <i>1.537 73–10</i> | 1.094 59–12 | 1.138 78–12 | <i>2.687 22–10</i> |
| 62 2.030 78–08 | 1.884 46–09 | 3.585 00–08 | 1.818 38–10 | 5.679 09–09 | 4.574 56–08 |
| | 3.366 27–10 | 1.216 48–10 | 4.651 79–10 | 3.015 43–11 | 2.699 22–10 |
| | 4.481 18–10 | | | | |
| <i>8.702 42–11</i> | 5.061 86–13 | <i>2.007 02–10</i> | 8.590 24–13 | 6.155 96–13 | <i>3.551 46–10</i> |
| 63 2.123 60–08 | 2.180 30–09 | 3.696 49–08 | 2.436 91–10 | 6.464 00–09 | 4.615 48–08 |
| | 2.868 29–10 | 1.102 88–10 | 3.834 54–10 | 2.910 50–11 | 2.373 69–10 |
| | 3.505 35–10 | | | | |
| <i>1.125 29–10</i> | 2.911 00–13 | <i>2.625 03–10</i> | 6.521 44–13 | 2.804 86–13 | <i>4.730 03–10</i> |
| 64 2.211 19–08 | 2.509 15–09 | 3.786 75–08 | 3.218 0–10 | 7.304 37–09 | 4.598 57–08 |
| | 2.408 31–10 | 9.895 93–11 | 3.088 98–10 | 2.789 31–11 | 2.046 49–10 |
| | 2.630 97–10 | | | | |
| <i>1.457 69–10</i> | 1.464 45–13 | <i>3.455 25–10</i> | 4.728 57–13 | 9.553 73–14 | <i>6.397 43–10</i> |
| 65 2.292 60–08 | 2.875 75–09 | 3.849 73–08 | 4.203 02–10 | 8.178 2–09 | 4.497 26–08 |
| | 1.985 97–10 | 8.762 06–11 | 2.414 37–10 | 2.640 78–11 | 1.713 26–10 |
| | 1.856 32–10 | | | | |
| <i>1.898 57–10</i> | 5.956 39–14 | <i>4.604 33–10</i> | 3.200 84–13 | 1.803 21–14 | |
| 66 2.366 50–08 | 3.284 65–09 | 3.875 22–08 | | | |
| | 1.600 87–10 | 7.618 61–11 | 1.809 79–10 | | |
| | <i>2.498 29–10</i> | 1.652 49–14 | <i>6.269 60–10</i> | | |
| 67 2.430 79–08 | | | | | |
| | 1.252 58–10 | | | | |

Quadrupole oscillator strength are presented in Figure 2, 3 and 4. All the points connected by a curve corresponds to transitions with the same value of the initial v_i and final v_f vibrational quantum number. For all the cases there is a systematic grouping of the curves depending of the difference between of the vibrational quantum numbers. Roughly the oscillator strength with $v_i - v_f = 1$ are larger by an order of magnitude than those with $v_i - v_f = 2$ and $v_i - v_f = 2$ are larger by an order of magnitude than those with $v_i - v_f = 3$.

Lifetimes for all states considered are calculated with

$$\tau = \left(\sum_{E_f < E_i} W_{i \rightarrow f}^{(2)} \right)^{-1}, \quad (3)$$

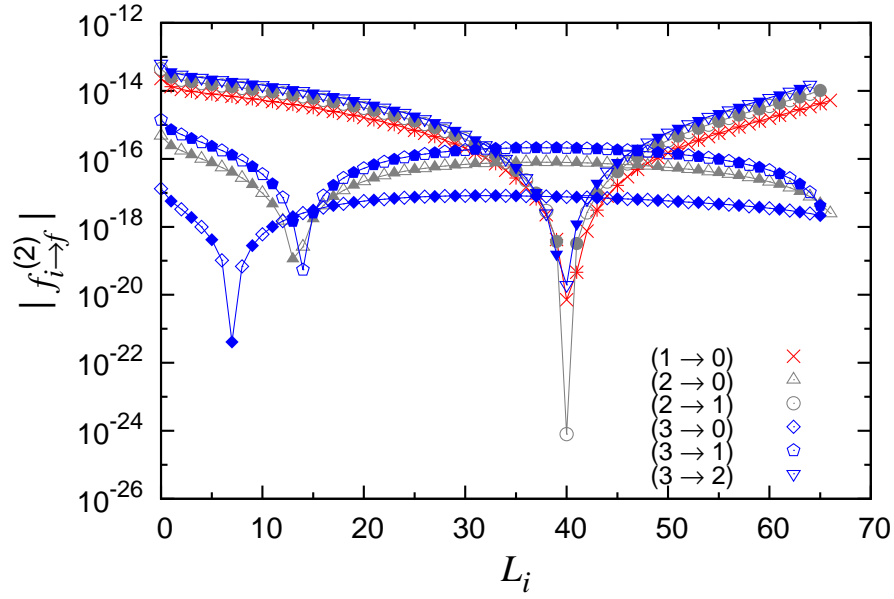


FIG. 2. Oscillator strengths for $L_f = L_i + 2$ transitions.

and are displayed in Figure 4. Using the allowed electric quadrupole transitions presented in tables II and III we obtain, for the vibrational states ($L = 0$) $v = 1, 2$ and 3: $\tau = 4.250\,039 \times 10^7$ s, $2.269\,525 \times 10^7$ s and $1.615\,861 \times 10^7$ s, respectively. The zero-vibrational states ($L^\pi, 0$) have the longer lifetime. Decreasing monotonically from $(2^+, 0)$ ($\tau = 777\,201$ years) up to $L \sim 25$. In this domain $L \in [0 - 25]$, the lifetime for the excited vibrational states $v = 1, 2, 3$ is around 9 months. For $L > 25$, the lifetime for all states decrease reaching a minimum around $L \sim 54$ ($\tau \sim 55$ days) and then starting to increase again slowly.

III. MASS DEPENDENCE

The mass dependence in the binding energy has been widely studied for three body Coulomb systems m_1 , m_2 and m_3 and in particular for the symmetric configuration where $m_1 = m_2$ (see for example [8] and [9] and references therein). The Lagrange-mesh method, briefly presented in section II, can easily be adapted to study the ground state energy of the symmetric three body systems with $m_1 = m_2 = m$ and m_3 . We consider the symmetric systems with one/two electrons: ${}^\infty\text{H}_2^+$ (infinite protons mass), $\text{Ps}^-(e^+e^-e^-)$, H^- , D^- , T^- , ${}^\infty\text{H}^-$ (infinite proton mass) and the muonic systems $\mu^+\mu^+e$ and μ^+ee . In the Lagrange-

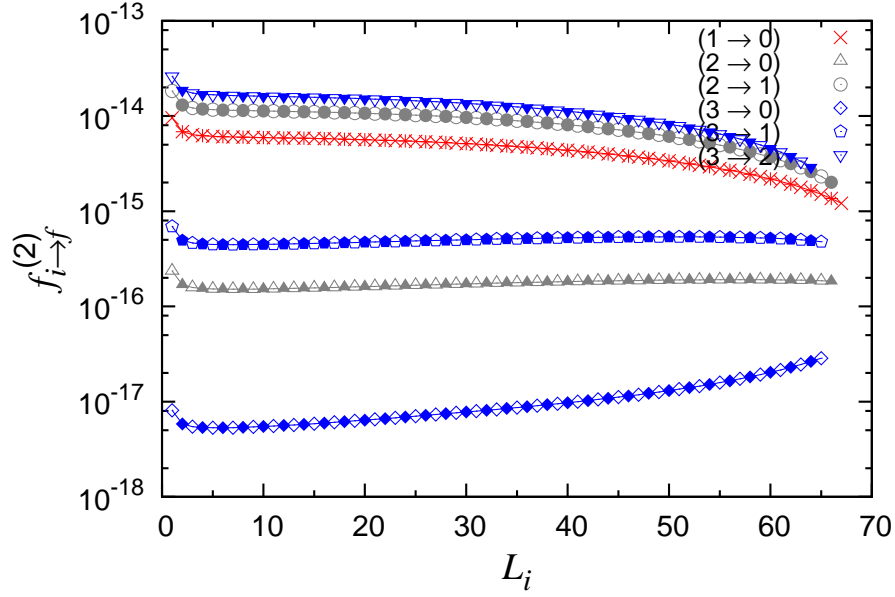


FIG. 3. Oscillator strengths for $L_f = L_i$ transitions.

mesh approach, energies and several properties of the systems Ps^- and ${}^\infty\text{H}^-$ were calculated in [10]. Results are presented in Table IV together with those of the molecular ion H_2^+ and its isotopomers D_2^+ and T_2^+ . The values, in atomic units, of the particle masses for the proton m_p , deuteron m_d , triton m_t and muon m_μ are

$$\begin{aligned} m_p &= 1836.152\,701, & m_d &= 3670.483\,014, \\ m_t &= 5496.921\,58, & m_\mu &= 206.768\,262. \end{aligned}$$

Following Gur'yanov and Rebane [8] the ground state energy is expanded as follows

$$E(\beta) \approx m\beta f(\beta), \quad (4)$$

where

$$f(\beta) = \sum_{j=0}^n C_j \beta^{j/2}, \quad (5)$$

and $\beta = m_3/(2m + m_3)$ varies between $[0, 1]$. The parameter C_0 is fixed in terms of the value of the ground state energy of the static hydrogen molecular ion ${}^\infty\text{H}_2^+$. First 5 terms in (4), $n = 5$ reproduce no less than 7 s.d. in energies with parameters

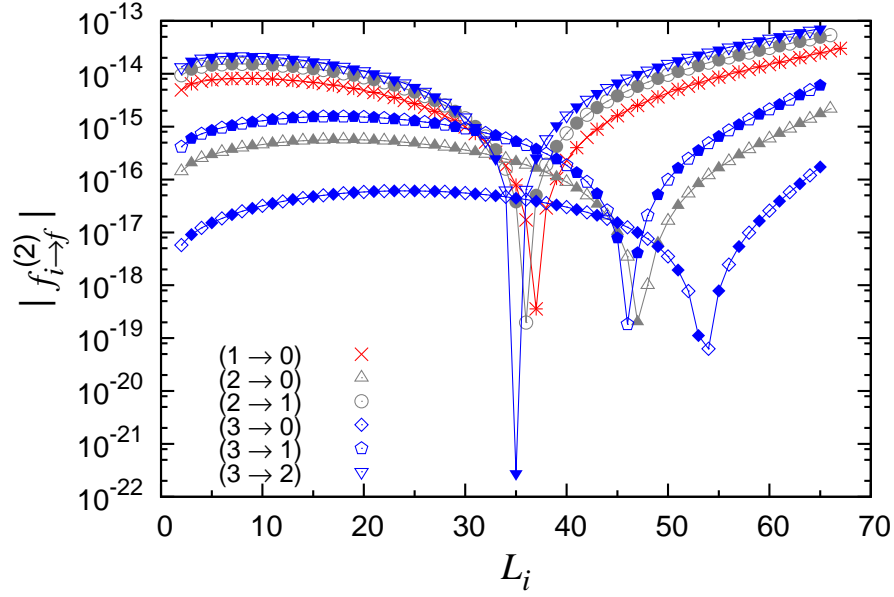


FIG. 4. Oscillator strengths for $L_f = L_i - 2$ transitions.

$$C_1 = 0.64179582, \quad C_2 = 0.28372246, \quad C_3 = -0.15304332, \\ C_4 = -0.21968058, \quad C_5 = 0.12472387,$$

which are in agreement to the parameters found in [8]. Increasing number of terms up to 7, we reproduce no less than 10 s.d. in energy (see Table IV) with parameters

$$C_1 = 0.64177988217, \quad C_2 = 0.28534422820, \quad C_3 = -0.18731634808, \\ C_4 = -0.04273755179, \quad C_5 = -0.24388850969, \quad C_6 = 0.33561102864, \\ C_7 = -0.11127450779.$$

The expansion $f(\beta)$ (5) is an increasing function of $\beta \in [0, 1]$ and is presented in Figure 6.

CONCLUSIONS

Summarizing, in order to solve the non-relativistic Schrödinger equation for the three body system with Coulomb interaction composed of two tritons and one electron, the Lagrange-mesh method is applied. The spectra for the four lowest vibrational states $v = 0, 1, 2, 3$ is presented with 13, 12, 11 and 10 significant digits using 54 mesh points in the $x - y$ perimetric coordinates and 18 mesh points in the z perimetric coordinate. It is found that

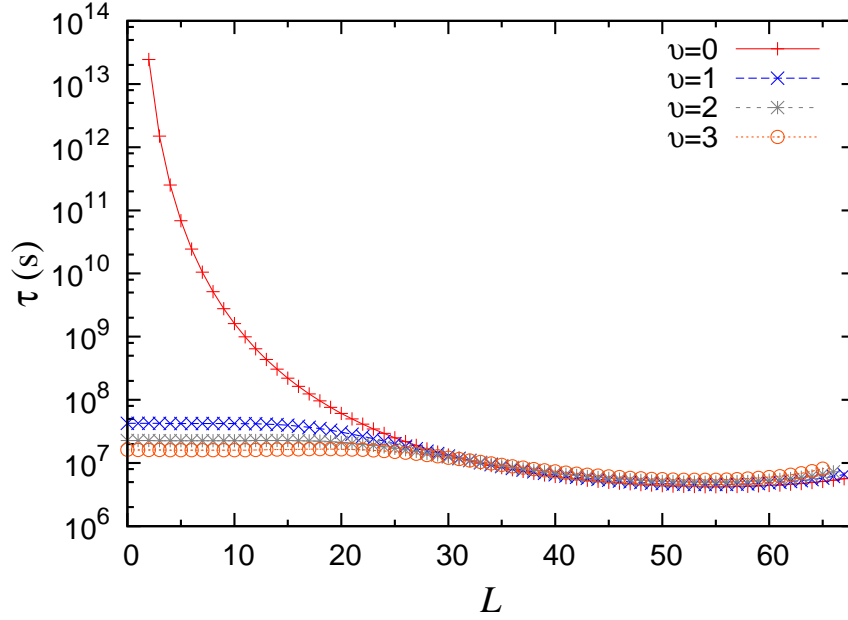


FIG. 5. Lifetimes in seconds for the first four rotational bands ($v = 0 - 3$).

the vibrational states $v = 0, 1, 2, 3$ support 62, 61, 60 and 58 rotational states, respectively. Some quasi bound states are also given. The vibrationless band $(L^\pi, 0)$ supports 27 (11) rotational bound states more than the isotopomer H_2^+ [5] (D_2^+ [6]). Table V presents a complete comparison between these systems.

Using the wave functions provided by the Lagrange mesh method it is easy to calculate the electric quadrupole transitions probabilities per second $W_{i \rightarrow f}^{(2)}$. All possible transitions probabilities are presented with six significant digits. Quadrupole oscillator strength $f_{i \rightarrow f}^{(2)}$ for $\Delta L = 2, 0, -2$ are depicted in Figures 2, 3 and 4, respectively. For $L_i = 41$ and beyond the $(L_i, 1) \rightarrow (L_i + 2, 0)$ transitions are replaced by $(L_i + 2, 0) \rightarrow (L_i, 1)$ transitions. The rotational state L_i after which the initial and final states are exchanged for the three cases $v_{1 \rightarrow 0}$, $v_{2 \rightarrow 1}$ and $v_{3 \rightarrow 2}$ and comparison with the molecular ions H_2^+ and D_2^+ are shown in Table V.

Qualitatively the behaviour of the electric quadrupole transitions $W^{(2)}$ resembles to that of the electric quadrupole oscillator strength (see Figures 2, 3 and 4). Comparing with the

TABLE IV. Ground state energies for symmetric three body systems $m_1 = m_2 = m$ and m_3 with Coulomb interaction. $\beta = m_3/(2m + m_3)$. Results for H_2^+ and D_2^+ from ^a[5] and ^b[6]. The symbol "∞" stands for an infinitely heavy particle. Comparison is made with ^c[3], ^d[11], ^e[12], ^f[13], ^g[14], ^h[15], ⁱ[16], ^j[17] (rounded).

| System | m | β | E_t (present) | Reference |
|-----------------------|--------------|----------------------------|------------------------------------|--|
| $^\infty\text{H}_2^+$ | $^\infty$ | 0.0 | -0.602 634 619 105 | |
| T_2^+ | 5496.921 58 | 9.0951729×10^{-5} | -0.599 506 910 111 5 | -0.599 506 910 111 541 ^c |
| D_2^+ | 3670.483 014 | 1.3620330×10^{-4} | -0.598 788 784 330 7 ^a | -0.598 788 784 330 68 ^d |
| H_2^+ | 1836.152 701 | 2.7223437×10^{-4} | -0.597 139 063 123 41 ^b | -0.597 139 063 123 405 ^e |
| $\mu^+\mu^+e$ | 206.768 262 | 2.4123327×10^{-3} | -0.585 126 097 219 20 | -0.585 126 097 219 193 ^f |
| Ps^- | 1.0 | 0.33333333 | -0.262 005 070 232 97 | -0.262 005 070 232 980 ^g |
| μ^+ee | 1.0 | 0.99042000 | -0.525 054 806 243 53 | -0.525 054 806 243 526 ^h |
| H^- | 1.0 | 0.99891195 | -0.527 445 881 114 18 | -0.527 445 881 114 179 ⁱ |
| D^- | 1.0 | 0.99945541 | -0.527 598 324 686 48 | -0.527 598 324 686 478 ⁱ |
| T^- | 1.0 | 0.99963629 | -0.527 649 048 203 01 | -0.527 649 048 202 999 95 ⁱ |
| $^\infty\text{H}^-$ | 1.0 | 1.0 | -0.527 751 016 544 38 | -0.527 751 016 544 377 ^{i,j} |

TABLE V. Comparison between the isotopomers H_2^+ , D_2^+ and T_2^+ . a) Number of rotational bound states for the lowest three vibrational states and b) rotational state after which the initial and final states are exchanged.

| | | | Rotational bound states | | | | Change direction | | |
|----------------|--------------|----------------------|-------------------------|---------|---------|---------|-----------------------|-----------------------|-----------------------|
| Mass | $(0^+, 0)$ | | $v = 0$ | $v = 1$ | $v = 2$ | $v = 3$ | $v_{1 \rightarrow 0}$ | $v_{2 \rightarrow 1}$ | $v_{3 \rightarrow 2}$ |
| H_2^+ | 1836.152 701 | -0.597 139 063 123 3 | 35 | 34 | 33 | 31 | 23 | 23 | 22 |
| D_2^+ | 3670.483 014 | -0.598 788 784 330 7 | 51 | 49 | 48 | 47 | 33 | 33 | 32 |
| T_2^+ | 5496.921 58 | -0.599 506 910 111 5 | 62 | 61 | 60 | 58 | 41 | 41 | 40 |

isotopomers H_2^+ [5] and D_2^+ [6] the hierarchy

$$W_{\text{H}_2^+}^{(2)} > W_{\text{D}_2^+}^{(2)} > W_{\text{T}_2^+}^{(2)}, \quad (6)$$

is found, except at some points near to the minima and at the ends of the curves. As a consequence, the lifetimes of T_2^+ are larger than those of D_2^+ and H_2^+ , around three times

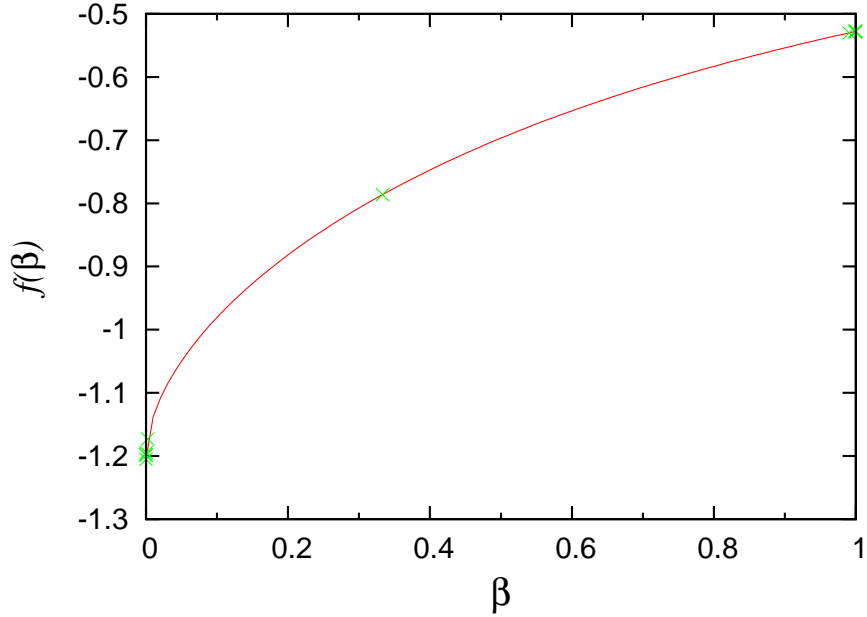


FIG. 6. Expansion $f(\beta)$ (5) for $n = 7$ (line). Symbols indicate all 11 systems present in Table IV.

and 21 times, respectively.

In order to study the mass dependence for the ground state of three body systems, we consider the systems $^{\infty}\text{H}_2^+$, $^{\infty}\text{H}^-$, Ps^- , H^- , D^- , T^- , $\mu^+\mu^+e$, μ^+ee and those previously investigated H_2^+ and D_2^+ (see Table 4). Expanding the energy as (4) and keeping 7 terms, $n = 7$, we reproduce no less than 10 s.d.

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